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Reduction of Uncertainties in Time - Dependent Complex Systems*

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Accurate prediction is the goal of every scientific theory. Predictability is permanently challenged by inherent uncertainties at the theoretical and experimental level alike. There are several potential approaches to uncertainty analysis. Response surface methods are a popular paradigm because of their intrinsic conceptual simplicity. Other techniques frequently used include fuzzy logic and cross validation. The methodology we address here is based on concepts and tools from *sensitivity analysis.* Sensitivities are defined as the derivatives of the system responses with respect to parameters and inputs. They are used to determine and rank the importance of model parameters and input data to computed quantities of interest (usually referred to as system responses), and to assess model uncertainties due to uncertainties in parameters and data.

Our uncertainty analysis methodology possesses five *key capabilities*. First, no *important effects* are overlooked, i.e., a *full set of sensitivities* is made available. A full set means that sensitivities with respect to all parameters are computed, without making an *a-priori* judgment as to which one is important. Second, an *efficient computation of the sensitivities* is implemented. For that purpose, adjoint operator methods and/or automated differentiation preprocessors can be considered. Third, our approach allows for a systematic treatment of *nonlinearities.* The fourth capability addresses the rigorous treatment, where relevant, of full *time dependence.* This includes model responses and (as needed, current and time-delayed) inputs and parameters. Finally, we consistently combine experimental (i.e., measured) data and model results, the primary goal being to *reduce the uncertainties* in the predicted model responses. In particular, we seek *best estimates* for the parameters and responses. This is achieved by optimizing a constrained Bayesian loss function, which simultaneously minimizes the differences (*i*) between the best estimate and the measured responses and (*ii*) the best estimate and the nominal values of the system parameters. Our optimization process uses the inverse of a global covariance matrix as the natural metric.

This paper describes the algorithms underlying our uncertainty analysis methodology, and presents results for (*i*) the *MODTRAN* code, which models radiation transport in the atmosphere, and (*ii*) for the *DeepNet* signal analysis code.

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